IN THE CLAIMS[1]

Please amend claims 19-23 as follows:

19. (Five Times Amended) A method of using a computer for evaluating the ability of at least one of a plurality of chemical entities to associate with a molecule or molecular complex comprising a calcineurin A (CnA) binding pocket defined by structure coordinates of CnA amino acids 90, 91, 92, 118, 120, 121, 122, 150, 151, 156, 160, 199, 232, 253, 254, 256, 281, 282, 283, 284, 306, 311, 312, and 317 according to Figure 1, or a homologue of said molecule or molecular complex wherein said homologue comprises a CnA homologue binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å;

wherein said computer comprises a machine-readable data storage medium comprising a data storage material encoded with said structure coordinates defining said binding pocket and wherein said method comprises the steps of:

a) utilizing said structure coordinates defining said binding pocket and the structure coordinates of one of said plurality of chemical entities to position a chemical entity within the CnA binding pocket or the CnA homologue binding pocket;

b) performing a fitting operation between said chemical entity and the CnA binding pocket or the CnA homologue binding pocket by employing computational means which utilize said structure coordinates of the binding pocket or the chemical entity ;

c) analyzing the results of said fitting operation to quantify the association between said chemical entity and the CnA binding pocket or the CnA homologue binding pocket;

d) optionally repeating steps a) through c) with another of said plurality of chemical entities; and

[1] An "Appendix of Amendments" is attached herein. In the Appendix, deleted portions of the claims are bracketed and added portions are underlined.

e) selecting at least one of said plurality of chemical entities that associates with the CnA binding pocket or the CnA homologue binding pocket based on said quantified association of said chemical entity.

20. (Five Times Amended) A method of using a computer for evaluating the ability of at least one of a plurality of chemical entities to associate with a molecule or molecular complex comprising a CnA binding pocket defined by structure coordinates of CnA amino acids 90, 91, 92, 118, 120, 121, 122, 150, 151, 156, 160, 199, 281, 282, 283, 306, 311, 232, and 254, according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a CnA homologue binding pocket that has a root mean square deviation from the backbone atoms of said amino acids of not more than 1.5Å;

wherein said computer comprises a machine-readable data storage medium comprising a data storage material encoded with said structure coordinates defining said binding pocket and wherein said method comprises the steps of:

a) utilizing said structure coordinates defining said binding pocket and the structure coordinates of one of said plurality of chemical entities to position a chemical entity within the CnA binding pocket or the CnA homologue binding pocket;

b) performing a fitting operation between said chemical entity and the CnA binding pocket or the CnA homologue binding pocket by employing computational means which utilize said structure coordinates of the binding pocket or the chemical entity ;

c) analyzing the results of said fitting operation to quantify the association between said chemical entity and the CnA binding pocket or the CnA homologue binding pocket;

d) optionally repeating steps a) through c) with another of said plurality of chemical entities; and

e) selecting at least one of said plurality of chemical entities that associates with the CnA binding pocket or the CnA homologue binding pocket based on said quantified association of said chemical entity.

21. (Five Times Amended) A method of using a computer for evaluating the ability of at least one of a plurality of chemical entities to associate with a molecule or molecular complex comprising a CnA/CnB binding pocket defined by structure coordinates of CnA amino acids 122, 124, 159, 160, 310, 312, 313, 314, 339, 341, 343, 344, 345, 347, 351, 352, 353, 354, 355, 356, 359, 360, and 363; and calcineurin B (CnB) amino acids 49, 50, 114, 115, 118, 119, 121, 122, 123, 124, 157, 158, 159, 161, and 162 according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a CnA/CnB homologue binding pocket that has a root mean square deviation from the backbone atoms of said CnA and CnB amino acids of not more than 1.5Å; wherein said computer comprises a machine-readable data storage medium comprising a data storage material encoded with said structure coordinates defining said binding pocket and wherein said method comprises the steps of:

a) utilizing said structure coordinates defining said binding pocket and the structure coordinates of one of said plurality of chemical entities to position a chemical entity within the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket;

b) performing a fitting operation between said chemical entity and the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket by employing computational means which utilize said structure coordinates of the binding pocket or the chemical entity;

c) analyzing the results of said fitting operation to quantify the association between said chemical entity and the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket;

d) optionally repeating steps a) through c) with another of said plurality of chemical entities; and

e) selecting at least one of said plurality of chemical entities that associates with the CnA/CnB binding pocket or the CnA/CnB homologue binding pocket based on said quantified association of said chemical entity.

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22. (Thrice amended) The method according to claim 19 or 20, wherein said molecule or molecular complex further comprises a second binding pocket defined by

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CnA amino acids 122, 124, 159, 160, 310, 312, 313, 314, 339, 341, 343, 344, 345, 347, 351, 352, 353, 354, 355, 356, 359, 360, and 363; and CnB amino acids 49, 50, 114, 115, 118, 119, 121, 122, 123, 124, 157, 158, 159, 161, and 162; according to Figure 1, or a homologue of said molecule or molecular complex, wherein said homologue comprises a second homologue binding pocket that has a root mean square deviation from the backbone atoms of said CnA and CnB amino acids of not more than 1.5Å.

23. (Thrice amended) The method according to claim 22, wherein said molecule or molecular complex is defined by the entire set of structure coordinates according to Figure 1, or a homologue thereof, wherein said homologue has a root mean square deviation from the backbone atoms of said CnA and CnB amino acids of not more than 1.5Å.

Please add claims 31-34 as follows:

31. The method according to any one of claims 19, 20 and 21 prior to step a), further comprising the steps of:

a) producing a crystal of a molecule or molecular complex comprising CnA/CnB;

b) determining the three-dimensional structure coordinates of the molecule or molecular complex by X-ray diffraction of the crystal; and

c) identifying said binding pocket.

32. The method according to any one of claims 25, 26 and 27 prior to step a), further comprising the steps of:

a) producing a crystal of a molecule or molecular complex comprising CnA/CnB;

b) determining the three-dimensional structure coordinates of the molecule or molecular complex by X-ray diffraction of the crystal; and

c) identifying said binding pocket.

33. The method according to any one of claims 19, 20 and 21 wherein the fitting operation utilizes energy minimization, shape complementarity or molecular dynamics.

34. The method according to any one of claims 19, 20 and 21 wherein the fitting operation is performed through visual inspection on a computer screen using a computer program capable of generating a three-dimensional graphical representation of said structure coordinates and structure coordinates of said chemical entity.